Acetic acid, (hexyloxy)-
57931-25-6 | DTXSID9069211

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -2.17 °C

Global applicability domain: Inside

Local applicability domain index: 5.64e-01

Confidence level: 7.37e-01

Nearest Neighbors from the Training Set

Image not found
9-Cycloheptadecen-1-one
Measured: 32.5
Predicted: 26.0

Image not found
Pentanoic acid
Measured: -34.0
Predicted: -30.1

Image not found
Hexanoic acid
Measured: -3.00
Predicted: -17.7

Image not found
Isovaleric acid
Measured: -29.3
Predicted: -29.1

Image not found
Pentanoic acid, 4-methyl-
Measured: -33.0
Predicted: -16.4